

A deformable elastic membrane embedded in a lattice Boltzmann fluid

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Abstract. A method is described for embedding a deformable, elastic, membrane within a lattice Boltzmann fluid. The membrane is represented by a set of massless points which advect with the fluid and which impose forces on the fluid which are derived from a free energy functional with a value which is dependent upon the geometric properties of the membrane. The method is validated in two dimensions with a free energy functional which imposes the constraint of constant membrane length, constant enclosed area, a bending rigidity and a preferred curvature. The method is shown to recover the expected equilibrium shape in the absence of flow and deformation in the presence of an applied shear flow. The method may have applications in a number of mesoscopic simulations, including discrete models of blood cells.

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1. Introduction

A number of biological objects can be represented as vesicles formed by polymerised membranes (Alberts *et al* 2002, Lipowsky 1991). While the conformations of such vesicles are determined by the elastic properties of the membrane (Lipowsky 1991), their dynamics in a flowing fluid is altered by the flow of the fluid outside and inside vesicles. Both factors should be taken into account in simulation of the membranes immersed into fluid host.

The lattice Boltzmann (LB) method (Succi 2001) provides a convenient method for introducing fluid flow in the presence of boundaries. An extension of the LB method to model fluid membranes in which the molecules rapidly diffuse within the membrane has been reported (Stelitano and Rothman 2000). However, this method cannot be straightforwardly generalised to the polymerised membranes since it does not allow for the extensional elastic properties which would be associated with such a membrane. An alternative approach is to model the membrane as a geometric object immersed into the LB fluid and this is the method adopted in this paper. A similar approach has been developed for the simulation of a polymer chain in an LB solvent (Ahlrichs and Dünweg 1998).

The aim of the present paper is to develop an LB method for the polymerised membranes. The main purpose of the paper is methodological and we therefore demonstrate the effectiveness of the method for a simple two-dimensional case. However, we discuss the generalisation to three dimensions in section 5. It is important to note that the motivation for the work in this paper is ultimately to develop models for flows in which there are embedded a large number of deformable membranes; this will form the basis of modelling blood flow at the veinule scale. For this reason, the finer details of the membrane properties are ignored (*eg* membrane dissipation).

The paper is organised as follows. In section 2 the method for introducing the membrane into the LB scheme is described. The explicit expressions for the forces arising from the membrane are derived in section 3. The results of the simulations of the relaxation of a closed membrane to its equilibrium state without and with shear flow are presented in section 4. Conclusions and possible extensions and applications are discussed in section 5.

2. Lattice Boltzmann

The basics of the LB method have been described in the literature (Succi 2001). The fluid in the LB method is considered as a field of the population densities $f_i(\mathbf{r}, t)$, which indicate the amount of fluid present at the lattice site \mathbf{r} at the discrete time t and moving with the velocity \mathbf{c}_i associated with the i -th lattice direction. The models with n velocities on a simple cubic lattice of dimension d are usually referred to as $DdQn$. The LGBK algorithm may be represented by the equation

$$f_i(\mathbf{r} + \mathbf{c}_i \delta_t, t + \delta_t) = f_i(\mathbf{r}, t) + \frac{1}{\tau} (f_i^{(0)} - f_i) + G_i, \quad (1)$$

where δ_t represents the time step, τ controls the kinematic shear viscosity of the lattice fluid through the relation

$$\nu = \frac{2\tau - 1}{6}\delta_t, \quad (2)$$

and the ‘forcing’ term

$$G_i = \frac{1}{c_s^2} t_i c_{i\mu} F_\mu, \quad (3)$$

may be used to impress an external force F_μ , where c_s is the speed of sound and the t_i are determined to achieve isotropy of the fourth-order tensor of velocities and Galilean invariance. Note that the expressions (1)–(3) are independent of the spatial dimension.

Velocity moments give the lattice fluid’s density and momenta through

$$\rho = \sum_i f_i = \sum_i f_i^{(0)}, \quad (4)$$

$$\rho \mathbf{v} = \sum_i \mathbf{c}_i f_i = \sum_i \mathbf{c}_i f_i^{(0)}, \quad (5)$$

where the equilibrium distribution function $f_i^{(0)}$ is

$$f_i^{(0)}(\rho, \mathbf{v}) = t_i \rho \left[1 + \frac{\mathbf{v} \cdot \mathbf{c}_i}{c_s^2} + \frac{|\mathbf{v}|^2}{2c_s^2} + \frac{(\mathbf{v} \cdot \mathbf{c}_i)^2}{2c_s^4} \right]. \quad (6)$$

The form of the equilibrium distribution function (6) ensures that relations (4,5) are satisfied and also determines the nonviscous part of the momentum-flux tensor of the lattice fluid,

$$\Pi_{\alpha\beta}^{(0)} = \sum_i f_i^{(0)} c_{i\alpha} c_{i\beta} = c_s^2 \rho \delta_{\alpha\beta} + \rho v_\alpha v_\beta. \quad (7)$$

The membrane is represented by a discrete set of points corresponding to the equidistant values of a parameter s . The difference $\Delta s = s_{i+1} - s_i$ between the values of the parameter s for the consecutive points is chosen to be comparable with the distance between LB nodes.

The membrane is treated purely as a geometric object and, contrary to (Ahlich and Dünweg 1998), the points of the membrane always move with the velocity of the underlying LB fluid determined from equation (5). Generally, the position of the points does not coincide with the location of LB nodes, so a weighted average is used based on the velocities at the nodes which bound the lattice primitive cell in which the point is situated. The weight of the contribution from each node is taken to be proportional to the distance of the node from the membrane point under consideration. The geometric properties of the membrane determine the force that is in turn applied to the LB fluid according to equation (3). Again, as the location of the point generally does not coincide with nodes, the force is distributed amongst the same set of nodes in accordance with their distance from the point at which the force originates. The value of the force is determined in section 3.

It should be noted that a membrane represented in this way will not strictly conserve its internal mass, and will therefore be slightly permeable. However, since

we are modelling polymerised membranes which are themselves weakly permeable, this is not considered to be a serious defect in the approach.

3. Forces

We describe the shape of the membrane by the vector function $\mathbf{r}(s)$ having the components $x(s)$ and $y(s)$. We choose the parameter s so that for the undeformed membrane (without internal stress) s coincides with the arc length parameter l of the curve. The parameter s spans the interval $(0, L_0)$, L_0 being the equilibrium length of the membrane. In general, the length of the membrane is determined by the expression

$$L = \int_L dl = \int_0^{L_0} u(s) ds. \quad (8)$$

Here $dl = u(s)ds$ is the length element,

$$u(s) = \sqrt{x'^2(s) + y'^2(s)}. \quad (9)$$

If the membrane is stretched/compressed, the free energy increases. The excess free energy is

$$A_L[\mathbf{r}(s)] = \frac{\alpha}{2} \int_0^{L_0} (u(s) - 1)^2 ds, \quad (10)$$

α being the membrane compressibility. The free energy arising from the bending elasticity of the membrane can be taken in form (Canham 1970, Helfrich 1973, Evans 1974):

$$A_K = \frac{\kappa}{2} \int_L (K(\mathbf{r}) - K_0)^2 dl, \quad (11)$$

$K(\mathbf{r})$ being the curvature, K_0 being the preferred curvature and κ being the bending rigidity coefficient. The curvature can be represented as a function of the parameter s

$$K(s) = \frac{x'(s)y''(s) - y'(s)x''(s)}{u^3(s)}. \quad (12)$$

and hence we can write

$$A_K[\mathbf{r}(s)] = \frac{\kappa}{2} \int_0^{L_0} (K(s) - K_0)^2 u(s) ds. \quad (13)$$

The contribution to the free energy due to the surface tension is $A_S = \sigma L$, or

$$A_S = \sigma \int_0^{L_0} u(s) ds, \quad (14)$$

σ being the surface tension coefficient. The fluid is assumed to be compressible and the equilibrium two-dimensional ‘volume’ of the fluid enclosed by the membrane is taken to be V_0 . The excess pressure is

$$p = -\beta (V[\mathbf{r}(s)]/V_0 - 1), \quad (15)$$

where β is the fluid compressibility, and the ‘volume’ of the droplet $V[\mathbf{r}(t)]$ is the functional of the membrane shape

$$V[\mathbf{r}(s)] = \int_0^{L_0} y(s)x'(s) ds. \quad (16)$$

The free energy due to the fluid compressibility is

$$A_V = \int_{V_0}^V p dV \quad (17)$$

or, after integration,

$$A_V[\mathbf{r}(s)] = \frac{\beta}{2V_0} (V[\mathbf{r}(s)] - V_0)^2. \quad (18)$$

As a result, the free energy of the interface can be represented as a following functional of the membrane shape:

$$A[\mathbf{r}(s)] = A_L[\mathbf{r}(s)] + A_K[\mathbf{r}(s)] + A_S[\mathbf{r}(s)] + A_V[\mathbf{r}(s)], \quad (19)$$

where $A_L[\mathbf{r}(s)]$, $A_K[\mathbf{r}(s)]$, $A_S[\mathbf{r}(s)]$ and $A_V[\mathbf{r}(s)]$ are given by formulas (10), (13), (14), and (18), correspondingly.

The force \mathbf{F} from the element dl of the membrane is found as the variational derivative of the free energy, $\mathbf{F}(s) = -\delta A[\mathbf{r}(s)]/\delta \mathbf{r}(s)$, and can be represented in form

$$\mathbf{F}(s) = \mathbf{F}_L(s) + \mathbf{F}_K(s) + \mathbf{F}_S(s) + \mathbf{F}_V(s) \quad (20)$$

with the components

$$\mathbf{F}_L(s) = -\alpha \left(K(s) \mathbf{n}(s) + \partial^2 \mathbf{r} / \partial s^2 \right), \quad (21)$$

$$\mathbf{F}_K(s) = \kappa \left[\frac{1}{2} K(s) \left(K(s)^2 - K_0^2 \right) + \frac{d^2 K(s)}{dl^2} \right] \mathbf{n}(s), \quad (22)$$

$$\mathbf{F}_S(s) = -\sigma K(s) \mathbf{n}(s), \quad (23)$$

$$\mathbf{F}_V(s) = -\beta (V[\mathbf{r}(s)]/V_0 - 1) \mathbf{n}(s), \quad (24)$$

corresponding to the membrane compressibility, bending elasticity, surface tension and fluid compressibility. In formulas (21–24), $\mathbf{n}(s)$ is the unit vector normal to the membrane with the components $n_x(s) = y'(s)/u(s)$ and $n_y(s) = -x'(s)/u(s)$. The expression for the force (22) is equivalent to that in (Stelitano and Rothman 2000) after it has been noted that there is an error in the quoted result which arises because the authors do not correctly account for the change in the metric tensor of the surface during the minimisation of the free energy (Lishchuk and Care 2005). Equation (22) also includes an additional contribution due to the preferred curvature K_0 .

The functions $x(s)$ and $y(s)$ can be approximated by polynomials. We use the second order polynomials,

$$\begin{aligned} x(s) &= a_0 + a_1 s + a_2 s^2, \\ y(s) &= b_0 + b_1 s + b_2 s^2. \end{aligned}$$

In order to determine the coefficients a_k and b_k $\{k = 0, 1, 2\}$ at the i -th point of the discretised membrane, we require the values of the functions at this and two neighbouring points to coincide with the corresponding positions,

$$\begin{cases} x(s_{i-1}) = x_{i-1} \\ x(s_i) = x_i \\ x(s_{i+1}) = x_{i+1} \end{cases}, \quad (25)$$

This represents a system of equations for a_k , and there is an analogous system for b_k . The values of these coefficients give the explicit form of the functions $x(s)$ and $y(s)$ in the vicinity of each point s_i that can be used to find its derivatives up to the second order. We note that the force on a point is different from the force on an element dl by a factor $u(s)$.

4. Validation

The method described in this paper is intended as methodological; there are no experimental results available for a two dimensional system. The results we give below, demonstrate that the method behaves in a manner which is consistent with the expected behaviour of a two dimensional cell. The possible extension of the method to three dimensions is discussed in section 5.

The simulations in this section were run on D2Q9 100×100 lattice with the periodic boundary conditions. The basis velocity vectors of the D2Q9 lattice and corresponding values of t_i are presented in the table 1. The primitive cell used for averaging the velocities, and distributing the forces, was taken to be a primitive square cell of the lattice whose corners are lattice nodes. The value of the relaxation time $\tau = 0.8$ was used in the simulations. The surface tension coefficient and the preferred curvature of the membrane were set to zero. The equilibrium distance between the membrane points $\Delta s = 3.2$ was used, and a typical membrane included 50 – 100 points.

Table 1. The basis velocity vectors of the D2Q9 lattice and corresponding values of t_i .

i	\mathbf{c}_i	t_i
0	(0,0)	4/9
1	(1,0)	1/9
2	(0,1)	1/9
3	(-1,0)	1/9
4	(0,-1)	1/9
5	(1,1)	1/36
6	(-1,1)	1/36
7	(-1,-1)	1/36
8	(1,-1)	1/36

Figure 1 shows the equilibrium shapes of the vesicle for different values of the parameter Q defined as

$$Q = L_0/L_c, \quad (26)$$

L_c being the length of the circular membrane with the same enclosed area. The parameters are: $\kappa = 0.05$, $\alpha = 0.01$, $\beta = 0.2$. To provide the slight initial asymmetry, the initial shape of the droplet was an ellipse with half-axes 20 ± 0.2 .

It should be noted that the same equilibrium shapes can be obtained without the including the effect of the embedding fluid; this was confirmed as one of the validations of the simulation. However, the inclusion of the LB fluid is necessary in order to recover the dynamics of the relaxation to the equilibrium shape, as is shown in Figure 2 for $Q = 1.4$ and different values of the bending rigidity κ . The value of κ also influences the rate of relaxation which is demonstrated in Figure 3 by the time dependence of the mean square velocity of the LB fluid for different values of κ .

To investigate the behaviour of the membrane in the flow, a simulation was undertaken in which shear flow was applied to an initially spherical membrane. Figure 4 depicts the time evolution of the shape of the droplet, and Figure 5 shows the velocity field of the LB fluid. Apart from the imposed shear, the parameters of the simulation are the same as in Figure 1 with the parameter Q was taken to be equal to 1.4. In the final steady state the membrane rotates with the fluid; however, this behaviour is expected only to occur in a two-dimensional system.

5. Conclusion

A method has been described for embedding a deformable membrane into a LB fluid and results presented which validate the approach in two dimensions. The method does not take into account thermal fluctuations. If the fluctuations are small they simply result in a renormalisation of the bending rigidity coefficient (Palmer and Morse 1996), and no further modification of the method is necessary. Large fluctuation can be taken into account by adding the random stress to the LB algorithm (Cates *et al* 2004).

The method could be generalised to three dimensions by employing the expression for the force due to bending rigidity of the two-dimensional membrane based on a corrected version of the result derived by (Stelitano and Rothman 2000) (see comment after equation (24)), and the method for calculating the curvature of the triangulated surface which has been developed by (Hamman 1993). Note that a grid would need to be created for the equilibrium shape of the membrane prior to LB simulation. This could be achieved by the direct numerical minimisation of the free energy of the membrane. After the minimisation, the equilibrium distances between points would be changed and the details of the area contributions would therefore need to be modified appropriately; work is currently in progress to implement such a three dimensional scheme.

One possible application of the technique described in this paper is a more accurate representation of the flow of blood cells in confined geometries and in which membrane elasticity effects are taken into account.

References

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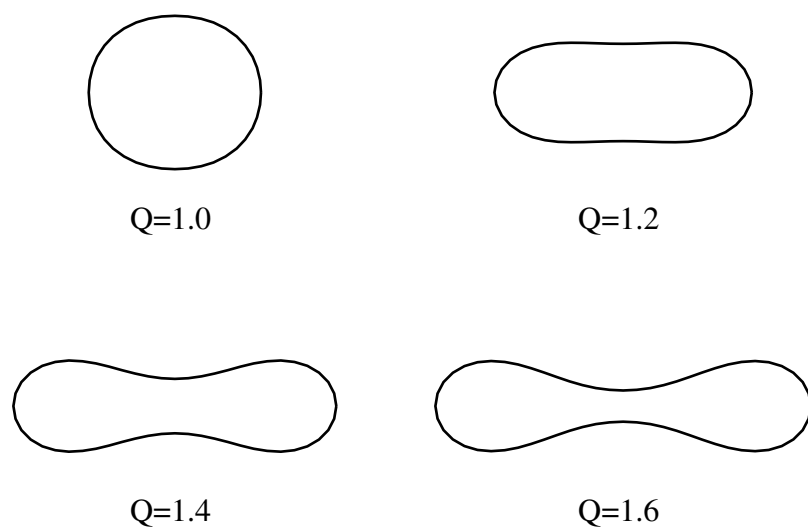


Figure 1. Equilibrium shapes for different values of the parameter Q defined by (26).

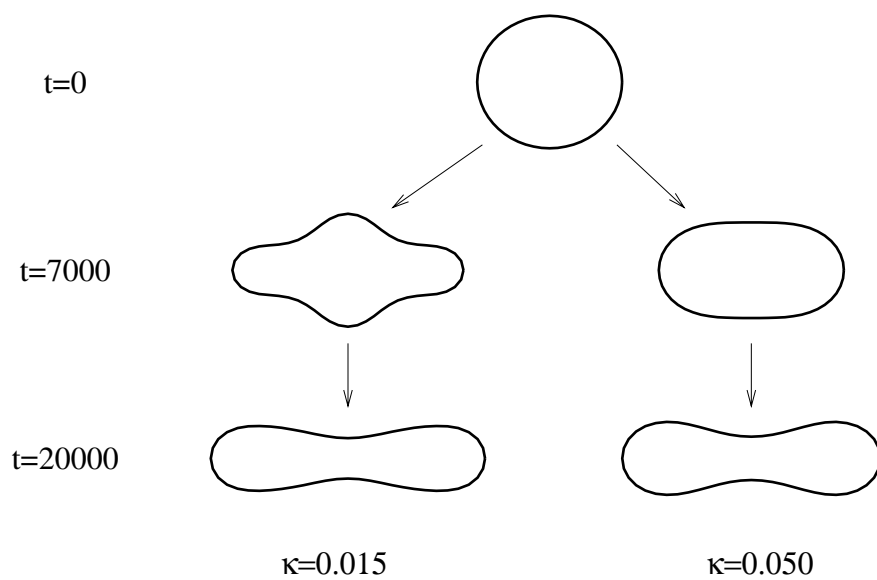


Figure 2. Dynamics for different values of the bending rigidity κ .

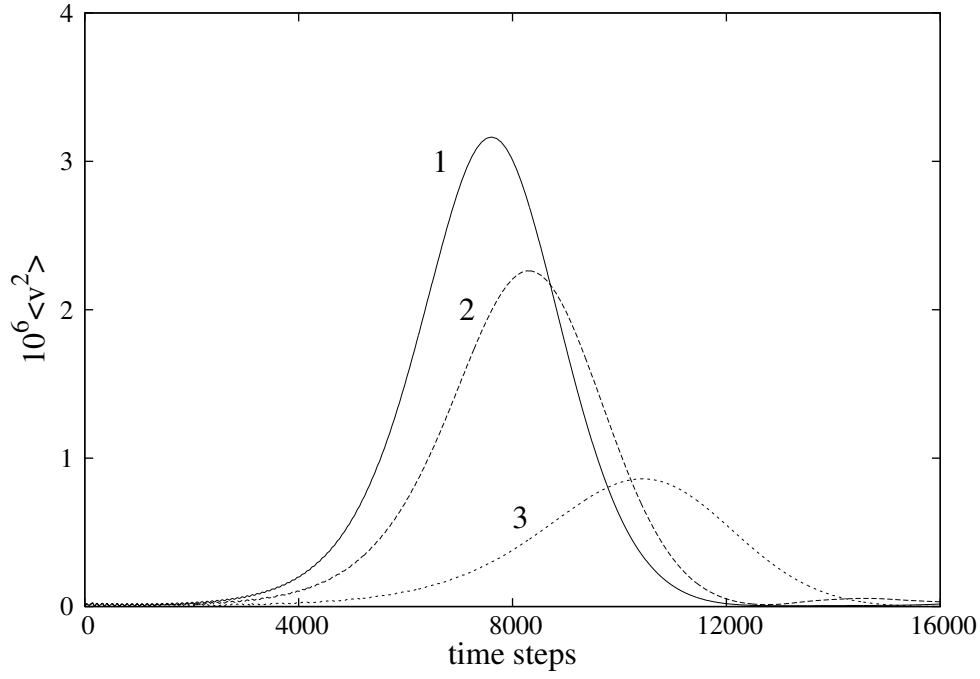


Figure 3. Time dependence of the mean square LB velocity for $\kappa = 0.025$ (curve 1), $\kappa = 0.05$ (curve 2), $\kappa = 0.1$ (curve 3).

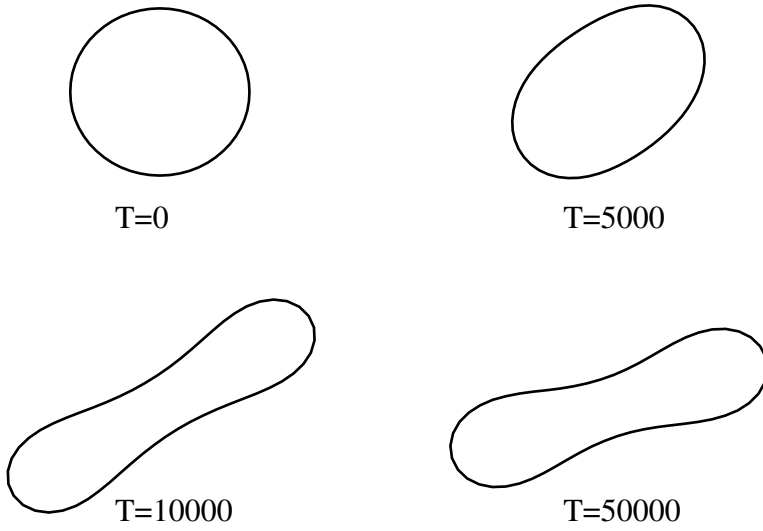


Figure 4. Dynamics of the membrane in shear flow.

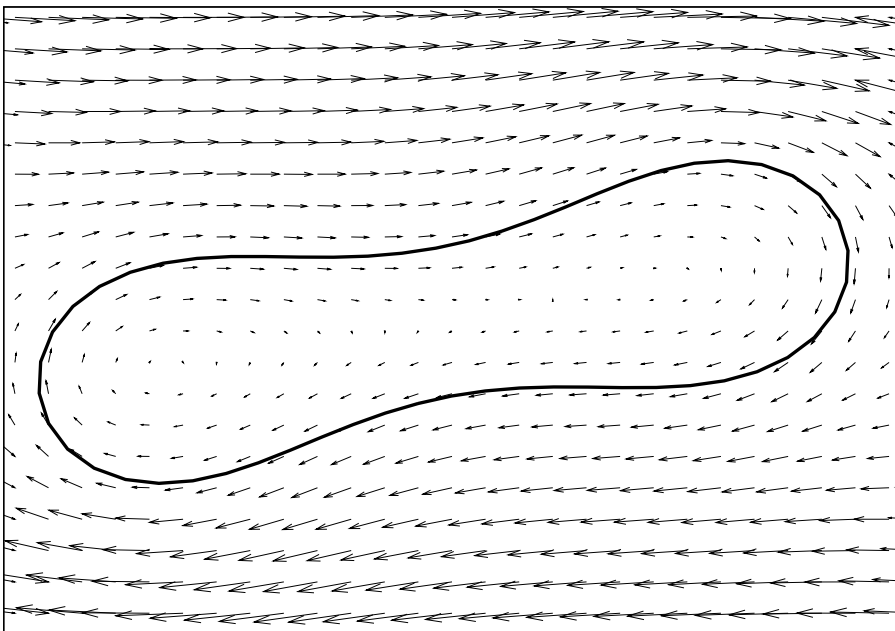


Figure 5. The velocity field of the LB fluid under shear.